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Photoionization cross section of the 6*s* electron of atomic cesium

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Abstract : The photoionization cross sections of the 6*s* electron of cesium atom are computed using independent particle model (IPM) potential of Green *et al* [*Phys. Rev.* **A184** 1 (1969)] (hereafter GSZ – IPM potential). The spin-orbit interaction is included in the model potential and the effects of core polarization are explicitly taken into consideration in both the model potential and the length form of the dipole transition matrix element. The variation of photoionization cross sections with photoelectron energy is in better agreement with relaxed-core results of Huang and Starace [*Phys. Rev.* **A19** 2325 (1979)] than their forzen-core results and also with the measurements of Cook *et al* [*Phys. Rev.* **A15** 1526 (1977)] upto about 0.7 eV.

Keywords : Photoionization matrix element, core-polarization, spin-orbit interaction

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Several theoretical studies have contributed to the increased understanding of spin-orbit interaction and core polarization effects in the photoionization of atomic cesium. Norcross [1] computed the ground state photoionization cross sections of atomic cesium using a semiempirical model potential having two adjustable parameters. Weisheit [2] also investigated this problem with core polarization correction to the dipole transition moment and spin-orbit perturbation of valence *p*-orbitals. Beigman *et al* [3] employed a semiempirical potential incorporating core polarization explicitly and also allowing for fine structure. Chang and Kelly [4] have obtained the photoionization cross section of cesium atom using Dirac-Fock wave function that itself includes the spin-orbit interaction. Huang and Starace [5] have presented the atomic Cs-photoionization cross section taking proper account of the final spin-orbit interaction. Jonson and Soff [6] have developed a relativistic many body method that takes into account correlation effect in the open shell atoms and strong spin-orbit effects found in Cs.

All these studies indicate that the spin-orbit calculation and the core polarization phenomena are important in investigating photoionization cross section of cesium atom. In the present study, we employ GSZ-IPM potential [7]. Such a potential has been very effective in calculating wave functions and also during the studies of ionization with different atoms. The single-particle wave functions resulting from the calculations with the GSZ-IPM potential have been used successfully to obtain one-electron energies for occupied orbits, electron-elastic scattering cross section, electron excitation cross section, ionization cross section, inner-shell ionization processes and optical oscillator strengths [8]. Even in the case of atomic Li photoionization [9], we noted that this GSZ-IPM potential has been a suitable choice to investigate the problem at low photon energies. Considering these findings, we investigate the photoionization of the 6*s* electron of cesium atom incorporating the effect of spin-orbit interaction and the core polarization effect both.

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The working formula for the photoionization cross section is adopted from the description given by McDowell [10]. When the effect of the spin-orbit perturbation of the free state photoelectron wave function is considered, there are two slightly different wave functions for the two final j values (1/2 and 3/2) with corresponding matrix elements M_1 and M_3. On taking the length-form of the photoionization matrix element, the expression for the total photoionization cross section (including the final state spin-orbit interaction) is given by

$$a_v = 0.856\,(I + K^2)\left(1/3\,M_1^2 + 2/3\,M_3^2\right) \quad \text{(in Mb)}, \quad (1)$$

where I and K^2 are the ionization potential of the atomic Cs and the kinetic energy of the photoelectron respectively (both given in Rydberg units). Here M_1 and M_3 are

$$M_1 = \int_0^\infty P_{6s}(r)\,Q(r)\,P_{k,\,1/2}(r)\,dr \quad (2)$$

and

$$M_3 = \int_0^\infty P_{6s}(r)\,Q(r)\,P_{k,3/2}(r)\,dr. \quad (3)$$

Here, $P_{6s}(r)$ is the ground state radial wave function of cesium and $P_{kP}(P = 1/2 \text{ and } 3/2)$ are the radial wave functions for the continuum states. In eqs. (2) and (3), $Q(r)$ is the corrected operator due to Weisheit following the core polarization correction to the one electron dipole transition matrix and is used in place of the operator r. $Q(r)$ is, however, taken to be

$$Q(r) = r\left[1 - \frac{\alpha_d}{r^3}\left(1 - \exp\,-\left(\frac{r}{r_c}\right)^3\right)\right], \quad (4)$$

where r_c is an effective core radius cut off and α_d is the static dipole core polarizability. The values of α_d and r_c for Cs atom are taken from the Table 1 of Hansen [11].

The normalized ground state wave function is taken from the tables of McLean and McLean [12] while the continua are numerically generated using Numerov procedure [13] by solving the following Schrödinger equation in an IPM approximation [7].

$$\left[\frac{d^2}{dr^2} + K^2 - \frac{2}{r^2} + V(r)\right]P_{kP}(r) = 0. \quad (5)$$

The potential $V(r)$ in which the radial part of the free state wave functions $P_{kP}(r)$ is constructed is the sum of the GSZ–IPM potential (V_g), the core polarization potential (V_P) and the spin-orbit interaction potential (V_{so}),

i.e.,
$$V(r) = V_g(r) + V_P(r) + V_{so}(r). \quad (6)$$

The GSZ–IPM potential [7] is given by

$$V_g(r) = \frac{2(N-Z)}{r}\left[(Z-1)\left(H\left(e^{r/d} - 1\right) + 1\right)^{-1} + 1\right], \quad (7)$$

where Z is the number of nuclear protons, N is the number of core electrons, r is the radial distance from the nucleus, d and H are the adjustable parameters. The polarization of the core by the valence electron is represented by the following model potential [11].

$$V_P(r) = \frac{\alpha_d}{r^4}\left[1 - \exp\left(-r/r_c\right)^6\right] + \frac{(\alpha_q - 3\beta a_o)}{r^6}\left[1 - \exp - \left(r/r_c\right)^{10}\right] \quad (8)$$

where α_q is quadrupole polarizability. $\beta\,(= 19.18\,a_0^4$ for Cs) is the nonadiabatic correction of the core polarizability, and a_o is the Bohr radius. The Dirac form of the spin-orbit potential [11] is taken to be

$$V_{so}(r) = \tfrac{1}{2}\alpha^2\,\frac{1}{r}\frac{d}{dr}\left(V_P + V_g\right) \times\left[1 + \frac{\alpha^2}{4}\left(V_P + V_g\right)\right]^{-2} \quad \text{(L.S.)}. \quad (9)$$

Here, α is the fine-structure constant. The term in the bigger bracket in eq. (9) is an additional relativistic correction to account for the proper behaviour of the spin-orbit interaction near the origin.

The numerically generated continua are normalized by Stewart's method [14]. If the unnormalized solution initially obtained in the asymptotic region is written as $P'(r)$ such that

$$\frac{P'(r)}{N} = P(r), \quad (10)$$

where N is the normalization constant.

Then
$$N = 1/2\left[(a_1 + a_2)^2\sec^2\alpha + (a_1 - a_2)^2\,\mathrm{cosec}^2\alpha\right]^{1/2}, \quad (11)$$

where
$$a_1 = \pi^{1/2} Z_1^{1/2} P'(r), \quad (12)$$

$$a_2 = \pi^{1/2} Z_2^{1/2} P'(r_2), \quad (13)$$

$$\alpha = \tfrac{1}{2}\int_{r_1}^{r_2} Z\,dr, \quad (14)$$

$$Z^2 = \lambda - \frac{1}{\lambda}\left(\frac{1}{r3} - \frac{3}{r4}\right) + \frac{1.25}{\lambda^2}\left(\frac{2}{r3} - \frac{1}{r2}\right)^2 \quad (15)$$

and

$$\lambda = K^2 - \frac{2}{r} + \frac{2}{r}. \quad (16)$$

Special care is taken to avoid those values of α which are equal or even very close to $n\pi/2$ and $(2n+1)\pi/2$ where n is an integer. For this, the lower limit r_1 and the upper limit r_2 of the eq. (14) are adjusted until the good values of α are obtained. The integration involved in the normalization of continua is done by Gauss quadrature rule. A finer initial radial interval (dr = 10^{-6} Å) is employed to ensure the accuracy in the numerical integration of the matrix element by the Simpsom quadrature rule. The computer program has been so designed and adjusted that the radial interval dr continues to be doubled each time after every 2000 steps until a considerable radial distance of about 40 Å is covered. The contribution beyond this radial distance is found to be negligible.

Our calculation for the photoionization cross section of the 6*s* electron of atomic cesium is shown in Figure 1.

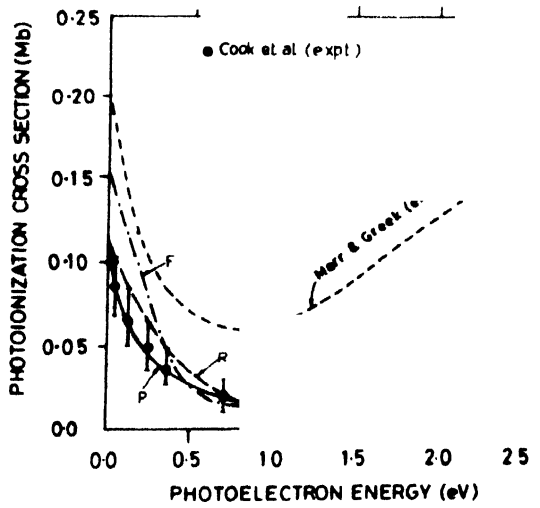

Figure 1. Photoionization cross section of the 6*s* electron in cesium *vs* photoelectron energy (eV)

Curve P : Present calculation

Curve F : Frozen-core results of Huang and Starace [5] in dipole-length approximation.

Curve R : Relaxed-core results of Huang and starace [5] in dipole-length approximation

● : Experimental results of Cook *et al* [15]

- - - - - : Experimental results of Marr and Greek [16].

All curves (except curve P) are taken from the Figure 2 of Ref. [5].

In fact, there are differences in the results between the different sets of the photoionization cross section calculations of the 6*s* electron of Cs atom due to Huang and Starace [5] (their all calculations not shown here) and also between two sets of experimental results [15,16]. In the figure, however, we have obly plotted their frozen-core (F) and relaxed-core (R) calculations both in the dipole-length approximation for comparison with our calculation. For photoelectron energies in the range between 0 and about 1.6 eV, the present results are in better agreement with the relaxed-core results of Huang and Starace than their frozen-core ones. Similarly for the photoelectron energies in the range between about 0.5 and 1.0 eV, an agreement of present results with their frozen-core results is also noticeable. The present calculation is in good agreement with the experimental measurements of Cook *et al* [15] only up to about 0.7 eV. In this energy region, the present caculations agree only qualitatively with the measurements of Marr and Greek [16] whose results are higher than ours by a factor of approximately 2. The present method, however, fails to yield the upward trend beyond about 1 eV as seen in the frozen-core calculations of Huang and Starace and also in both of these measurements. Considering the simplicity of the present method and agreement with measurements of Cook *et al* and also with calculations of Huang and Starace in the aforesaid energy range of the photoelectron, the present method is encouraging. The inadequacy of the present method at high photon energies has also been noticed in our earlier paper on atomic Li [9].

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